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Abstract:

Recently it was proposed that voids in crystals could grow by emission of shear dislocation loops [1]. Even more recently, this proposal was ostensibly supported by MD simulations of voids in strained single crystals [2]. The purpose of this comment is to dispute this recent assertion as unfounded.

Keywords:

Void growth, Dislocation nucleation, Dislocations, Molecular dynamics

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A common definition of shear (slip) loops can be found in the textbooks on crystal dislocations. For example, on page 151 in [3], a shear loop is defined as "… one with its Burgers vector lying in the loop plane". This has to be contrasted with prismatic loops commonly defined, according to the same source [3], as ones for which "… the Burgers vector is not in the plane of the loop." In [1,2] the authors adhere to the same common definitions and insist that the loops formed in their proposed void growth mechanism are shear and not prismatic.

In general, the amount of material that has to be removed or inserted to create a dislocation loop is equal to

$$\delta V = \int_{Surface} \mathbf{b} \cdot d\mathbf{A} = \int_{Surface} (\mathbf{b} \cdot \mathbf{n}) dA \ , \qquad (1)$$

where the integral is taken over an arbitrary surface bounded by the loop, **b** is the loop's Burgers vector, dA is the differential surface element and **n** is the unit normal to the surface at the location of surface element $d\boldsymbol{A}=\boldsymbol{n}dA$ [4][1]. In particular, material content in a shear loop is zero since $\mathbf{b}\cdot\mathbf{n}=0$ for any shear loop by definition. Thus, growth or shrinkage of voids by emission or absorption of shear loops violates mass conservation. Although this should be sufficient to invalidate the mechanism proposed in [1], in view of its recent high visibility [5] here we review the initial justification [1] and the later evidence presented in its support [2,5-7].

First, we observe that atomistic simulations reported in [2,5-7] present no evidence for the emission of complete shear loops. It stands to notice that material content expressed in (1) is defined only for a closed loop whereas the atomistic configurations shown in figures 7-12 and 14 in [2], figures 6 and 8 in [5], figures 1 and 2 in [6] and figures 4, 5, 6 and 7 in [7] contain no closed loops but only dislocation lines connected to the void surface. To define the material content integral (1) it is necessary to define a closed loop first. For an incipient loop connected to the void, this requires to identify a step on the void surface that connects two dislocation exit points and completes the loop. Each incipient line coming off the loop surface leaves behind (carves) a surface step whose local height h_s is equal to the scalar product of the Burgers vector and the local normal to the void surface, $h_s = \boldsymbol{b}\cdot\boldsymbol{n}$. Integral (1) is zero for any incipient loop that is formed by conservative dislocation motion (glide, shear, slip) and closed by the surface steps it carves on the void surface. This net zero value of the integral means that combined material content of the "void + step + incipient loop" agglomerate remains the same as before, even if material may have redistributed between the "void+step" and the incipient loop. It is only after the incipient loop detaches from the void that the material content of the loop and the void can be separately evaluated using

[1] The same expression can be used to compute material content of any dislocation agglomerate (tangle, network) that is *closed*, i.e. not connected to any other crystal defect. This can be done by deconstructing the network into constituent loops, computing the integral expression (1) for each loop and summing up the results.

expression (1). No such analysis was presented in [1,2] and in subsequent publications by the same group of authors [5-7].

The incipient loops observed in MD simulations [2,5-7] come off the void surface along two intersecting {111} glide planes in the form of leading and trailing partial dislocations that indeed appear different from schematic depictions of prismatic loops prevalent in the literature. Yet, the observed evolution is precisely equivalent to the early stages of the textbook mechanism of prismatic loop emission detailed, for example, in figure 8.3 on page 166 in [3]. The confusion possibly stems from the shapes of the observed incipient loops that are markedly stretched along the glide cylinder. However, the mass content and, hence, the loop character – shear or prismatic – are invariant with respect to an arbitrary distortion of the loop along the glide cylinder. Figure 1 sketches the sequence through which an elongated incipient shear loop transforms into two prismatic loops, in the reaction "shear loop" = "surface indent" + "prismatic loop". It is the same textbook mechanism as in [3] but our schematic is slightly modified to show the preferred {111} glide planes and dislocation dissociations in FCC crystals observed in [2,5-7]. Although rationally possible, emission of complete shear loops is extremely unlikely under deformation conditions reported in [2,5-7] given that the trailing segments of the shear loops (the steps) are pulled back towards the void surface by the image forces and by the same shear stress that presumably pulled the leading segments out of the void. Exceedingly more likely is that, once fully developed, the incipient shear loop will transform into a pair of prismatic loops, just like in the standard mechanism sketched in Figure 1.

Second, the initial justification given in [1] for void growth by shear loop emission is based on pictorial illustrations that are either irrelevant or geometrically flawed. In particular, the 2d schematic of dislocation emission given in figure 9 in [1] and reproduced here in Figure 2, is appropriate to illustrate dislocation emission from a cylindrical void but not from a spherical void in 3d. Furthermore, the dashed lines drawn on Figure 2(a) and Figure 2(b) to contrast shear and prismatic loops are used inconsistently: in Figure 2(a) the lines show the extra planes of atoms contained between two dislocations in each dipole while in Figure 2(b) the lines track the planes along which dislocations move away from the cylindrical void. If the lines were to be used for the same purpose or altogether removed, it would be obvious that the configurations shown in Figures 2 (a) and Figure 2(b) are identical.

The original 3d schematic given in figure 6(b) in [1] and reproduced here in Figure 3 is *escheresque*: two circular steps (rims) on the void surface can not be formed as shown, i.e. by the emission of shear loops. Instead, assuming the same incipient shear loops as in Figure 3, the void configuration should be as depicted in Figure 4(a) below, where each incipient loop is connected to its own surface step so that the loops are closed along the void surface. Should the shear loops actually detach from the void (this is extremely unlikely), the surface steps would disappear and the void would return to its precise initial shape as before loop emission (Figure 4(b)). It was argued later [2] that a circular step on the void surface of the kind sketched in

Figure 3 can be produced by simultaneous emission of six ½<110> edge dislocations in a single {111} plane intersecting the void. However, even if such an exotic rosette configuration were to form under stress, it would remain forever connected to the void by six radial dislocations. The realistic mechanism by which a void can grow is the familiar one: the emitted dislocations lines should eventually join, through cross-slip, to form a prismatic loop that can then detach and move away from the void surface (Figure 1).

To clear up the recent confusion concerning the role of shear loops in void growth it may be useful to place findings reported in [1,2,5-7] in the context of other relevant studies, both recent and old. Production of prismatic loops by conservative (shear, slip) dislocation motion is not at all unusual and have been proposed and observed in a variety of situations. Assorted examples of such mechanisms can be found in the literature, including obstacle by-passing by double cross-slip [8], formation of prismatic debris in dislocation intersections [9, 10], jog-dragging [11], cross-kinks and roughening of screw dislocations [12,13], etc. In all cases, dislocation cross-slip leads to the development of three-dimensional dislocation configurations and eventual line reconnection producing prismatic loops (or individual vacancies or interstitials).

The incipient shear loops observed in [2,5-7] appear to be nothing but the early stages of the standard mechanism depicted in Figure 1. This particular mechanism of prismatic loop emission by shear loop expansion and cross-slip was first detailed 40 years ago in [14] and later analyzed in atomistic details in [15]. Similar incipient shear loops were observed in most other recent MD simulations [16-19]. The same simulations confirmed that eventual formation of prismatic loops is a necessary and unavoidable stage of void growth [17]. Short of prismatic loop emission, the incipient (shear) loops remain attached to the void surface and disappear when the stress subsides [19]. In some conditions multiple incipient shear loops with different Burgers vectors come off the void surface simultaneously or in a rapid succession resulting in dislocation reactions and dense tangles that can survive even after the stress is removed [19]. However, for as long as the tangles remain connected to the void, the resulting defect agglomerate, while more topologically complex, contains exactly the same amount of material as the initial void.

Concerning the details of void expansion and its synchronization with dislocation activity, void expansion is a continuous process and some of it takes place before the prismatic loops form, i.e. while the incipient shear loops are still expanding and cross-slipping [17]. Void expansion then proceeds continuously as prismatic loops pinch off and move away from the void and completes only after the emitted prismatic loops run away to infinity [20]. If and when the stress is removed or reduced, even a fully formed prismatic loop can move back and become reabsorbed by the void under the action of attractive image forces [21]. Hence, the critical stress required to render loop punching and void expansion permanent must be higher than the stress required to initiate the first stage of void expansion, i.e. emission of incipient shear loops [20].

In summary, even if the incipient dislocations observed in MD simulations [2,5-7] were to develop into complete shear loops (an extremely unlikely scenario), their emission would have no effect on the resulting void volume. There is little doubt however that, once fully detached from the void, the incipient loops would transform into prismatic ones rendering the mechanism observed in [2,5-7] unremarkable.

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Figures

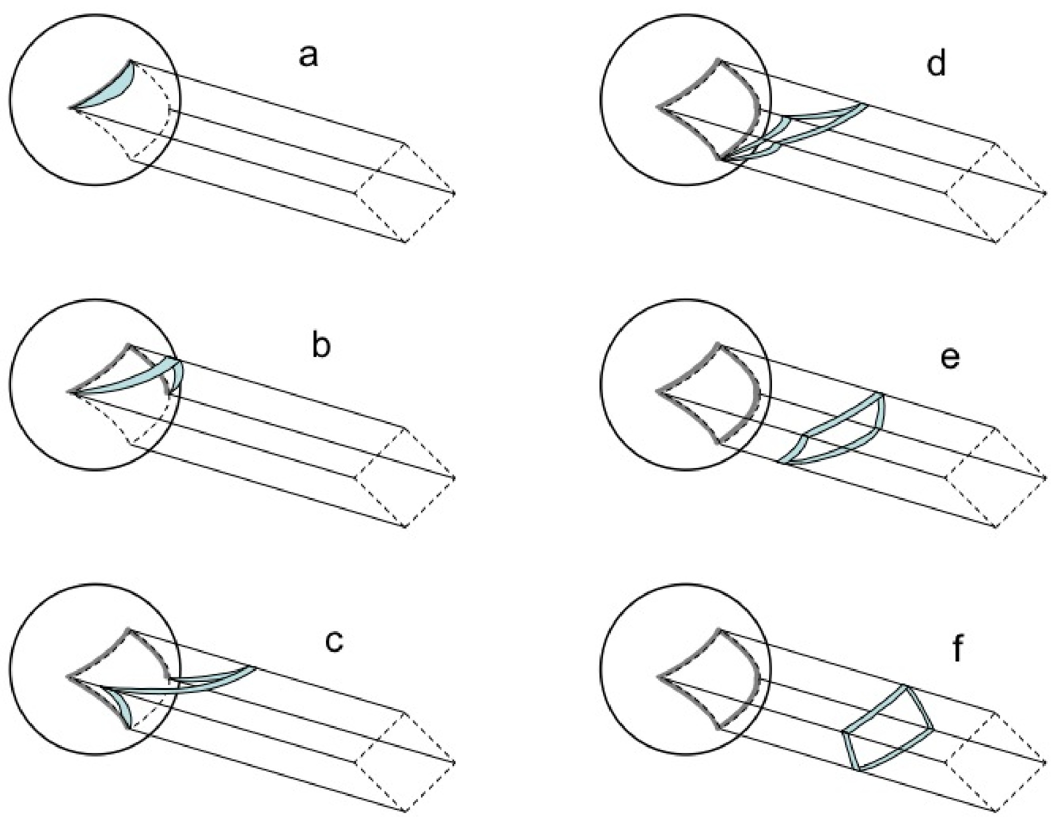

Figure 1: A sequence by which prismatic loops can be emitted from a void in an FCC crystal. Stages (a-b) can be observed in MD simulations reported in [2,5-7]. Subsequent emission of additional dislocations on the intersecting {111} planes (c) produces a complete loop that detaches (d) and moves away from the void (e) gradually acquiring the shape commonly expected of a prismatic loop (f). The ribbons of stacking faults bounded by partial dislocations are shown in light blue. The dashed lines show the glide cylinder cross-section - a rhomb in this case - and its projection on the void surface. The thin solid lines are the edges of the glide cylinder along which the loop segments are connected by cross-slip. Once separated, the loop detaches from the void and leaves behind a depression on the void surface bounded by the surface steps shown as thick gray lines. The depth of this depression is equal to the Burgers vector.

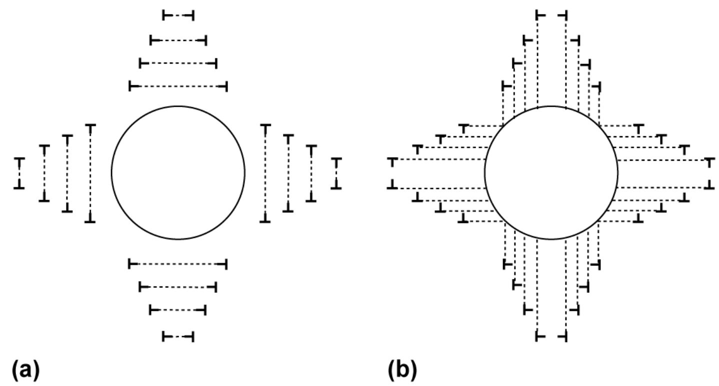

Figure 2: Reproduced from figure 9 in [1].

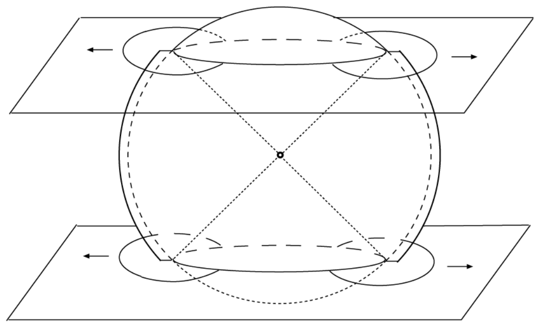

Figure 3: Reproduced from figure 6(b) in [1].

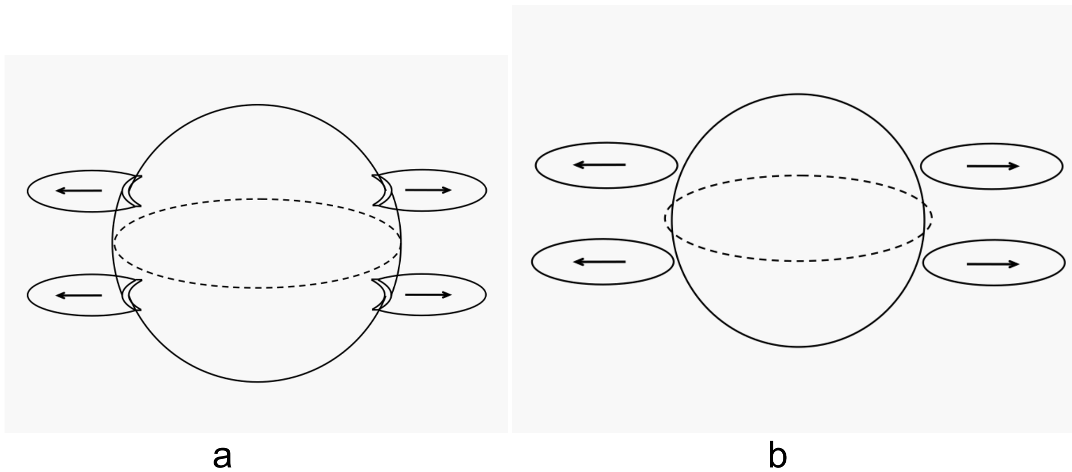

Figure 4: (a) Four incipient shear loops are connected to the steps on the void surface. (b) If the shear loops were to separate from the void, the void would return to its initial state and volume, as before loop emission.